

Quark Contraction Tool - QCT

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Abstract

We present a Mathematica package for the calculation of Wick contractions in quantum field theories - QCT. Furthermore the package aims at automatically generating code for the calculation of physical matrix elements, suitable for numerical evaluation in a C++ program. To that end commonly used algebraic manipulations for the calculation of matrix elements in lattice QCD are implemented.

1. Introduction

Matrix elements in lattice QCD are typically expressed as expectation values of time ordered products of quark operators, which can be computed by means of Wick contractions [1]. The aim of this package is to simplify and automate this straightforward but error prone task.

Currently only fermionic contractions are supported, i.e. the fields are assumed to be Grassmann valued. The complexity of the calculation grows as $N!$, where N is the number of creation or annihilation operators in the matrix element, i.e. the total number of quark field operators is $2N$. The contraction of 16 quark fields of identical type takes roughly 30 seconds¹ generating 40320 terms.

2. Basic functionality

The package provides functions to perform Wick contractions and subsequently simplify the expressions, i.e. contract indices and rewrite the results into QDP++ [2] mnemonics. For the Wick contractions the package expects fermionic field operators, where the fields have color and spin indices, and

¹Timings refer to a system with an Intel Core i5 running @ 2.6 GHz.

depend on the position. The creation (annihilation) operators are denoted by

```
Field{B}[<type>,<color index>,<spin index>,<position>]
```

The simplest contraction thus reads

$$f_{\mu}^a(x)\bar{f}_{\nu}^b(y) = S_{\mu\nu}^{ab}(y,x) \quad (1)$$

where the fermion propagator S of particles of type f connects point y to x . This contraction can be done within the package as

```
In[1]:=
WickContract[Field[f,a,mu,x]**FieldB[f,b,nu,y]]
Out[1]=
DE[{f, f}, {y, x}][CI[{a, b}], SI[{mu, nu}]]
```

where `**` is the builtin `NonCommutativeMultiply` operator, and `DE` denotes the propagator of a particle of type `f` with the color (spin) indices enclosed in the function `CI` (`SI`). The package defines formatting rules for certain expressions, i.e. in Mathematica's `TraditionalForm` or `TeXForm` the output is specially typeset, e.g. the color indices appear in the exponent and the spin indices are displayed as subscripts. The above expression in `TeXForm` reads

```
In[2]:=
TeXForm[DE[{f, f}, {y, x}][CI[{a, b}], SI[{mu, nu}]]]
Out[2]=
S_{\mu \nu }^{\{f,ab\}}(y,x)
```

There is a convenience function `ToQDP`, which rewrites the expressions in a format suitable for calculation within the `QDP++` [2] package. For the above term the conversion reads

```
In[3]:=
ToQDP[%]
Out[3] =
/*
Result is of type SpinColorMatrix
{S^f1(x1,y1) -> quarkProp1}
*/
quarkProp1
```

where in the comment section a description of the QDP++ type that is returned is given, together with a list of abbreviations for propagator objects. The abbreviations are not *canonical*, i.e. different expressions might give different abbreviations. Additionally one can provide a list of replacement rules as a second argument, e.g. special characters or sub-/superscripted quantities where the CForm would generate undesired terms. Furthermore the package provides the function `QuarkContract`, which performs a variety of manipulations to arrive at simpler forms, e.g. index summations

```
In[4] :=
  QuarkContract[WickContract[
    Pol[SI[{nu, mu}]] ** Field[f, a, mu, x] ** FieldB[f, b, nu, y]
  ]]
Out[4] =
  traceSpin[Pol . DE[{f, f}, {y, x}]] [CI[{a, b}]]
```

or more complicated substitutions including color contractions

```
In[5] :=
  QuarkContract[
    Eps[a, b, c] Eps[a', b', c'] Op[CI[{a, a'}], SI[{mu, nu}]] *
    Op'[CI[{b, b'}], SI[{mu, rho}]]
  ]
Out[5] =
  quarkContract[{1, 3}, Op, Op'] [CI[{c', c}], SI[{nu, rho}]]
```

where the `quarkContract[##]` function is defined within QDP++. Additionally we provide an `Uncontract` function, which will split contracted expressions into terms with open color and spin indices. Note that this function will introduce a color and spin index irrespective of the operator at hand, e.g. a color neutral object has superfluous color indices after the uncontract operation. We define δ functions to be independent of their index type and it suffices to write `DD[a,b]` = δ_{ab} .

3. Example applications

Let us illustrate the capabilities of the package by means of two examples.

3.1. Λ Baryon

Suppose we are interested in the large time behavior of the matrix element

$$\mathcal{M} = \langle \mathcal{O}_\mu \overline{\mathcal{O}}_{\mu'} \rangle P^{\mu' \mu} \quad (2)$$

e.g. the two point function of a Λ baryon. Let us write the interpolating operator for the Λ baryon [3]

$$\mathcal{O} = \epsilon^{abc} \Gamma^A (2s_a(u_b^T \Gamma^B d_c) + d_a(u_b^T \Gamma^B s_c) - u_a(d_b^T \Gamma^B s_c)), \quad (3)$$

$$\overline{\mathcal{O}} = \epsilon^{abc} \left(2(\bar{u}_a^T \tilde{\Gamma}^B \bar{d}_b) \bar{s}_c + (\bar{u}_a^T \tilde{\Gamma}^B \bar{s}_b) \bar{d}_c - (\bar{d}_a^T \tilde{\Gamma}^B \bar{s}_b) \bar{u}_c \right) \Gamma^A, \quad (4)$$

where we used a vector notation, i.e. the operators have an open spin index. These operators in QCT read

```
In[6] :=
OP =
Eps[a, b, c] ** (Gamma^A)[SI[{mu, alpha}]] ** (2 **
Field[s, a, alpha, x] ** Field[u, b, beta, x] **
(Gamma^B)[SI[{beta, gamma}]] ** Field[d, c, gamma, x] +
Field[d, a, alpha, x] ** Field[u, b, beta, x] **
(Gamma^B)[SI[{beta, gamma}]] ** Field[s, c, gamma, x] -
Field[u, a, alpha, x] ** Field[d, b, beta, x] **
(Gamma^B)[SI[{beta, gamma}]] ** Field[s, c, gamma, x])

In[7] :=
OPBar =
Eps[a', b', c'] ** (2 **
FieldB[u, a', gamma', y] ** (Gamma^BT)[SI[{beta', gamma'}]] **
FieldB[d, b', beta', y] ** FieldB[s, c', alpha', y] +
FieldB[u, a', gamma', y] ** (Gamma^BT)[SI[{beta', gamma'}]] **
FieldB[s, b', beta', y] ** FieldB[d, c', alpha', y] -
FieldB[d, a', gamma', y] ** (Gamma^BT)[SI[{beta', gamma'}]] **
FieldB[s, b', beta', y] ** FieldB[u, c', alpha', y]) **
(Gamma^A)[SI[{alpha', mu'}]]
```

Within QCT the two point function can be computed as

```
In[8] :=
Timing[Contracted =
```

```

WickContract[P[SI[{mu', mu}]] ** OP ** OPBar];]
Out[8] =
{0.016128000000000142, Null}

```

where the result still has yet to be contracted spin and color indices. Note that the computational time is negligible for a matrix element comprised of 6 quark operators. Simplifying the expressions further

```

In[9] :=
Result = QuarkContract[Contracted];
ToQDP[
Simplify[Result], {Gamma^B -> GammaB, Gamma^A ->
GammaA, Gamma^BT -> GammaBT}]

```

gives the result

```

Out[9] =
/*
Result is of type Scalar
{S^d(y,x) -> quarkProp1, S^s(y,x) -> quarkProp2,
S^u(y,x) -> quarkProp3}
*/
trace(quarkContract13(quarkProp1,GammaB*quarkProp2*GammaBT)*
transposeSpin(GammaA*P*GammaA*quarkProp3))
+
2*trace(quarkContract13(quarkProp3,GammaB*quarkProp1)*
transposeSpin(GammaA*P*GammaA*quarkProp2*GammaBT))
+
trace(quarkContract13(quarkProp3,GammaB*quarkProp2*GammaBT)*
transposeSpin(GammaA*P*GammaA*quarkProp1))
+
2*trace(quarkContract13(GammaB*quarkProp2,quarkProp1*GammaBT)*
transposeSpin(GammaA*P*GammaA*quarkProp3))
.
.
.

```

The `QuarkContract` function, as shown in the previous section, contracts all open color and spin indices and identifies special patterns, e.g. resulting in QDP++ `quarkContract[##]`, `transposeSpin ...` function calls.

3.2. Sequential Source

Another illustrative example is a generic 3 point function

$$\mathcal{M} = \langle \mathcal{O} \mathcal{J} \overline{\mathcal{O}} \rangle \quad (5)$$

Let us assume the following operators, e.g. nucleon interpolating operators and a flavor preserving current, again adopting a vector notation,

$$\mathcal{O} = \epsilon^{abc} O^A u_a (u_b \Gamma^B d_c), \quad (6)$$

$$\overline{\mathcal{O}} = -\epsilon^{a'b'c'} \left(\bar{d}'_a \tilde{\Gamma}^B \bar{u}'_{b'} \right) \bar{u}'_c \tilde{O}^A, \quad (7)$$

$$\mathcal{J} = \bar{d} J d. \quad (8)$$

In QCT the operators, amended with explicit spin and color indices, read

```
In[10] :=
OP = Eps[a, b, c] ** OA[SI[{mu, alpha}]] **
Field[u, a, alpha, y] ** Field[u, b, beta, y] **
GammaB[SI[{beta, gamma}]] ** Field[d, c, gamma, y]

In[11] :=
OPBar = -Eps[a', b', c'] ** FieldB[d, a', alpha', x] **
GammaBT[SI[{alpha', beta'}]] ** FieldB[u, b', beta', x] **
FieldB[u, c', nu', x] ** OAT[SI[{nu', mu'}]]

In[12] :=
Jc = FieldB[d, f, sigma, z] ** J[sigma, rho] **
Field[d, f, rho, z]

In[13] :=
MatrixElement =
OP ** Jc ** OPBar ** P[mu', mu]
```

Now the matrix element can be parameterised as

$$\mathcal{M} = \Sigma(JS^d(z, x)) \quad (9)$$

where for the sake of readability we have omitted all volume sums and fourier modes. The term Σ is called the sequential propagator. The corresponding

source can be constructed using QCT, where one starts from the Wick contracted matrix element, projects out the part proportional to $(JS^d(z, x))$ and subsequently applies the Dirac equation to generate the sequential source - for a discussion of the technique see e.g. [4].

First to get the matrix element we write

```
In[14] :=
MatrixElementContracted =
WickContract[MatrixElement] /. DE[_, {a_, a_}][_] -> 0
```

where the replacement gets rid of disconnected pieces, i.e. propagators with identical start and end points. The package implements a projection operator `DEProject` for propagators, i.e.

$$S_{\nu_1, \nu_2}^{f, b_1, b_2}(x, z) \text{Proj}_{f, \mu_1, \mu_2}^{a_1, a_2}(x, z) = \delta_{a_1 b_2} \delta_{a_2 b_1} \delta_{\mu_1 \nu_2} \delta_{\mu_2 \nu_1} \quad (10)$$

$$\mathcal{M}(S^f(x, z)) \text{Proj}_{\mu_1, \mu_2}^{f, a_1, a_2}(x, z) = \mathcal{M}_{\mu_1, \mu_2}^{a_1, a_2}(x, z) \quad (11)$$

Thus the easiest way to project out the sequential propagator is to replace the current with a δ -function and project out the propagator connecting the source point x with the current insertion point z

```
In[15] :=
MatrixElementConnectedProj =
Expand[MatrixElementContracted] /.
J[sigma, rho] -> DD[rho, sigma];
```

```
In[16] :=
SeqProp =
Contract[Expand[
Uncontract[MatrixElementConnectedProj]
DEProject[{d, d}, {x, z}][CI[{a1, a2}], SI[{mu1, mu2}]]]]];
```

The expression `SeqProp` is equivalent to $\Sigma_{\mu_1 \mu_2}^{a_1 a_2}(x, z)$. Next to find the source that generates this propagator we multiply with the inverse Dirac propagator from the right, i.e.

$$\eta_{\mu_1 \mu_3}^{a_1 a_3}(x, y) = \Sigma_{\mu_1 \mu_2}^{a_1 a_2}(x, z) S_{\mu_2 \mu_3}^{-1, a_2 a_3}(z, y) \quad (12)$$

In QCT this reads

```

In[17] :=
  QuarkContract[
    Uncontract[Contract[SeqProp]]*
    DEInverse[{d, d}, {y, z}][CI[{a2, a3}], SI[{mu2, mu3}]]]

Out[17] =
  (quarkContract[{1, 4}, OAT . P . OA . DE[{u, u}, {x, y}] .
    Transpose[GammaBT], DE[{u, u}, {x, y}]] . GammaB)[CI[{a1, a3}],
    SI[{mu1, mu3}]] +
  (transposeSpin[quarkContract[{3, 4}, DE[{u, u}, {x, y}] .
    Transpose[GammaBT], OAT . P . OA . DE[{u, u}, {x, y}]]] .
    GammaB)[CI[{a1, a3}], SI[{mu1, mu3}]]

```

Note that to obtain the sequential source we applied the Dirac operator from the right

$$\sum_y \Psi(y) S^{-1}(y, x) = \eta(x) \quad (13)$$

Usually lattice QCD codes implement a solver, where the solution from point x to point y

$$\sum_y S^{-1}(x, y) \Psi(y) = \eta(x) \quad (14)$$

is calculated applying the Dirac operator from the left. Rewriting Eq.(13)

$$\sum_y S^{-1}(y, x)^\dagger \Psi(y)^\dagger = \eta(x)^\dagger \quad (15)$$

$$\sum_y S^{-1}(x, y) \gamma_5 \Psi(y)^\dagger = \gamma_5 \eta(x)^\dagger \quad (16)$$

one can however easily construct the sequential propagator using *ordinary* solves.

4. Summary

The aim of the package is to simplify the straightforward but error prone task of computing matrix elements in QCD. To that end we implemented routines that perform Wick contractions on quark operators, further simplify the

results and write out QDP++ expressions directly calculable within a C++ program. Since the results are automatically generated, in most cases, manual fine tuning will be necessary to obtain the most efficient implementation of the matrix element at hand. Nevertheless QCT is, at the very least, useful to check the correctness of the implementation. The code is open source [5].

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References

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